Visual Simulation Tools: Solutions to Shift the Education Paradigm

Judith Light Feather, President, The NanoTechnology Group Inc.

Advances in microscopy and optical lenses have opened the 'window to nature' allowing us to see how the world actually works at the atomic level. This scale of science is all-encompassing and demands collaboration between physics, chemistry, biology, engineering and information technology, along with simulation and modeling software technicians.

Our organization is constantly searching for solutions to provide more visual elements to include in the curriculum development for students to understand and work at the atomic scale of science. Most of the simulation programs are designed for the university level research students and professors. Some of the programs we have found are at the pre-launch testing phase, while others are ready for commercialization. All of the companies are offering large discounts and/or free trial offers for education and government use of the software. We have placed a few of them prior to this article on our website for access and have recently been introduced to several other new programs designed for specific areas of research in nano science.

All of the tools are necessary for the various focuses of research and study at the atomic level. It is imperative that visual simulation tools and programs are adopted into all education programs as viable solutions.

Introducing the first systems engineering software for nanodevice design

Recently, I was introduced to Vic Peña, CEO of nanoTITAN Inc., whose company has developed a systems engineering software for nanodevice design and communication. Mr. Peña has an excellent background in visualization tools from his years at TASC, a subsidiary of Northrup/Grumman. During our conversation he also stated that when he and his partner, Rob Bishop, nanoTITAN's CTO, left TASC, it became their largest client for the new software programs that are specific data visualization tools in myriad applications. These tools became the foundation for their flagship product, nanoXplorer™.

nanoTITAN was incorporated on January 19, 2001—at the dawn of the new millennium— in the Commonwealth of Virginia. According to Mr. Peña, their mission is to be the premier provider of software, information and services to the nanotechnology community and to assume a central role in the evolution of nanotechnology from basic research to profitable application: "Enabling the Diamond Age."

Since I was interested in visual simulation software for education, my first question was, "What level of student would this system be practical for in the area of education, or did you just design it for commercial applications in the industry?"

"Basically, we target students at the university level and especially those conducting research. However, it can also be adaptable for workforce technician training at

Community Colleges and maybe the few Advanced Technical High Schools who would like to develop an introductory level course", stated Peña.

"What if the graduate students that had the program in a university lab, could provide a few sample files of the early basic research from the program, which could then be developed into Introductory curriculum for high schools?, I inquired. "It may be an avenue to explore with universities who are using the system", replied Peña.

"What is the difference between your system for designing molecular devices and other simulation software that models molecular motors at the nanoscale" was my next question.

"Simulation programs are usually designed for specific purposes and the categories are so broad when involving chemistry, biology and physics at the nanoscale. Therefore, instead of working in a single focus area, we decided to tackle the issue of 'whole system thinking' software applications that can handle a research project from the first molecule to the prototype device stage for commercialization in materials science, hence our systems approach", stated Peña.

"Our philosophy is one of incremental growth in capability—'three yards and a cloud of dust,' if you will, which is why we are aiming at becoming the Nanoinformatics leader. If you take the whole systems approach from the beginning, the growth stems from the essential needs of an early stage industry's growth. Our software designs will incorporate that growth which all starts in the research labs at universities as well as governments and corporations," he explained. "You also must realize that our software is designed for all areas of research in materials science, so I recommend other programs to universities that are working on research of electrical nanoscale devices, such as Atomistix in Denmark. They excel in this area of electronics simulation software,"

"In conclusion, we are still the only simulation developer that has taken on the whole system approach, and materials science is a very important research area for nanoscale products entering the marketplace in this decade. Our nanoinformatics system will help move the current research and development of nanomaterials into the marketplace with an accurate prototype that will enhance the cost effectiveness of the commercialization process. This stage is a requirement for all research funding awarded to universities as government grants. Nanoinformatics includes the components that protect the Intellectual Property (IP) for the Patent process within the system for each research project creating an ecological economy from concept stage in the lab to market."

The components of Nanoinformatics

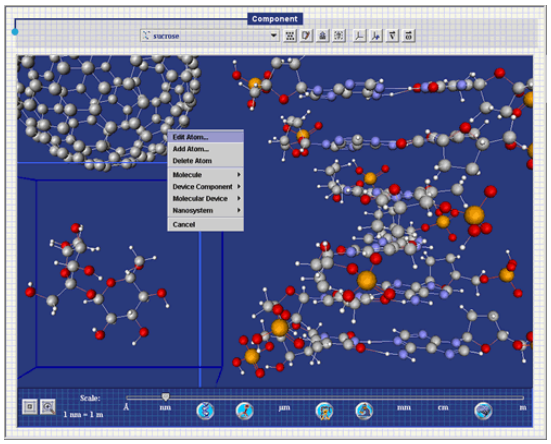
Nanoinformatics starts with nanoXplorer—the essential software resource for the nanotechnology workgroup. Researchers and engineers can use nanoXplorer to explore, exchange and engineer the full range of their nanodevice inspirations, from concept to commercialization. Built on the principles of life cycle systems engineering, nanoXplorer complements chemical analysis and simulation software by providing management of all aspects of a nanodevice. The user of this program is presented with in-depth information,

which includes the chemical structure, properties, operational characteristics, interface and connection details and visualizations of the molecular nanodevice.

While there is no “official” definition of “nanodevice,” in the nanoXplorer software it has the specific meaning of a molecular device, comprised by components with nanoscale dimensions that have a particular purpose or function. “Nanoscale” indicates a size ranging from a small molecule (each atom is about one tenth of a nanometer—or one Angstrom) to about 100 times larger than that, or the approximate size of typical virus. These are not strict thresholds in practice, but offer a good framework for a universal understanding of the scale involved.

An example of a very simple existing nanodevice is a carbon nanotube. Though only a single molecule, it can be used for a variety of purposes as a result of its unique properties. For example, it may be used as a component in electronics due to its ability to act as a conductor or semiconductor (depending on its configuration), it has incredible tensile strength making it ideal for reinforcing materials and can even emit photons under certain conditions, leading to its use in certain display technologies just coming to market. More complex examples of nanodevices can be found both in nature (for example, ion channels) and on the drawing boards of many leading edge laboratories.

nanoXplorer is the first software application to make the nanodevice its central paradigm In order to handle multiple levels of complexity, nanoXplorer models nanodevices as a hierarchical collection of components broken down into three levels.



The Component Toolbar provides easy access to all of the components that a user can include in a nanodevice. This includes all of the levels of the nanodevice model hierarchy: nanosystems, molecular devices, device components, molecules and volumes—as well as interfaces and connections. It also includes custom configuration tools for specific molecules of special interest to nanotechnologists: nanotubes, buckyballs, DNA and dendritic polymers.

Data Protection in the program

The digital rights feature enables a user to prohibit third parties from certain actions (display, edit, save, aggregate) as they pertain to a particular piece of the nanodevice design. Permission to perform those actions may be granted subject to certain constraints and requirements. Constraints may include a cap on the number of uses or sunrise/sunset times. Requirements may include the need to accept an agreement or make payment.

By enabling a system where information can be protected and offered for compensation, nanoTITAN is planting the seeds for e-commerce in nanodevice designs.

Intuitive Interactive 3D environment

The Structure Panel provides fine control over the structure of a nanodevice through an intuitive interactive 3D environment. It is very easy to add new atoms and bonds, or delete them—or even edit the atom type or bond order, in place. This interactivity feature makes this program one of the most advanced molecular design tools on the market, where molecular design is a crucial element of nanodevice design. The flexible Pattern Tool also allows a user to specify a rectangular, cylindrical or spherical pattern of objects. This can help the nanodevice designer quickly create large devices that have repeating elements.

Supported data types include nanodevice designs (nanoML), molecules (e.g., CML, PDB), trajectories, images, videos, numerical data files (NetCDF) and text files. Any data incorporated into the nanodevice design is saved along with it (in nanoML) and is available each time the nanodevice design is opened for viewing. Thus the Data Panel is a powerful tool for both analysis and collaboration. Simulated and experimental data can be easily organized and shared with peers. Helpful images, animations and miscellaneous files can accompany a design to make sure the essential design elements are not lost. Students and novices can come up to speed quickly.

The Operation Panel captures the functionality of the nanodevice being designed. Eight categories of operational capability are summarized in the display and may be edited by the user.

1. ***Chronometry*** *-- indicates the ability of the nanodevice to sense or keep time.*
2. ***Communication*** *-- indicates the ability to transmit and receive data.*
3. ***Computation*** *-- captures its suitability to be used as a component of a computational device.*
4. ***Energy*** *-- refers to its ability to convert energy from one type to another as well as its ability to generate power or requirement for power to operate.*
5. ***Motility*** *-- indicates its ability to move in various environments.*
6. ***Safety*** *-- is a consideration with nanodevices, particularly with regard to replication, environmental impact and biohazard.*
7. ***Sensing*** *-- captures the nanodevices ability to sense things about or in its environment.*
8. ***Transport*** *-- indicates whether the nanodevice can move other things.*

The Assembly Panel captures information about a Nanodevice's interfaces and (for a Nanosystem) the connections between subsystems. A nanodevice can have any number of interfaces, which in turn can have any number of “joins.” A “join” has a particular type (chemical, electromagnetic, physical or remote) and position.

The Display Panel captures visualizations of the nanodevice and can be used to convey important information to others that will view a nanodevice design. A standard 3D view

is always included, but the user can add additional 3D views as desired, with a high degree of flexibility in what is displayed. The user can also capture or load 2D images for inclusion in the nanodevice.

Analyzing Stability and Feasibility
The program includes molecular mechanics simulation for performing geometry optimization/ energy minimization for large molecules (such as molecular devices). This is useful for analyzing the structural stability and feasibility of a particular design. It also includes a fully-integrated version of the Nano-Hive Nanospace Simulator, a flexible open-source tool for analyzing the physical world at the nanometer scale. With Nano-Hive it is possible to calculate spatial and temporal properties of nanodevice components, including molecular trajectories that display atomic positions as a function of time. Nano-Hive can also perform electrostatic potential calculations of interest in many areas of nanotechnology. The simulation capabilities can be extended by wrapping any 3rd party simulation, simply by creating user interface and data handling components that adhere to nanoXplorer's simulation API.

Built in Language
NanoML is an XML-based markup language for specifying nanodevice designs. It includes the chemical structure of the nanodevice, but goes far beyond that to include properties and operational characteristics, visualizations, digital rights, interface information and more. As such it is the ideal vehicle for transmitting information about nanodevice designs to colleagues and the public in general. NanoML serves as the foundation file format for both nanoXplorer and the Nanodevice Database. NanoML is a registered trademark of nanoTITAN.

Included in the nanoXplorer programs are the following components:
nCyclopedia, a nanotechnology Wiki available on the nanoTITAN web site and **nCyclopedia Plus™**, an enhanced selection of news, articles and data for nanotechnology topics available exclusively from nanoXplorer 2005.

nVisualizer™, a powerful data visualization application that offers clients an easy to use tool for converting digital data into any combination of 3D, 2D and aural elements. Its component architecture allows rapid development of interactive information spaces. Open source Java™ libraries of general use to scientists, engineers and developers, including the popular Quantity LIbrary, which models numerous physical quantities, their units and operations. nanoTITAN is partnered with Nano-Hive™, incorporating its Nanospace Simulator technology into nanoXplorer 2005, leveraging its powerful and extensible simulation capabilities. nanoTITAN is partnered with TASC, Inc., a Northrop Grumman Company, to provide visualization.

Now educators and students can enter the nanoscale together with nanoXplorer 2005' Professional with features that enable 2-way collaboration between educators, colleagues and students providing real-time dynamic sharing of nanodevice designs and related data with licensing fees customized to your needs.

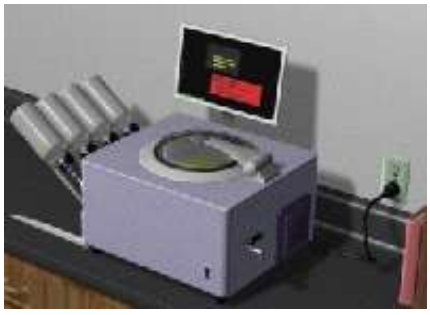
Education Discounts Available – Approx. 33% for universities and government use.

A Free test download is also available at:
www.nanoTITAN.com

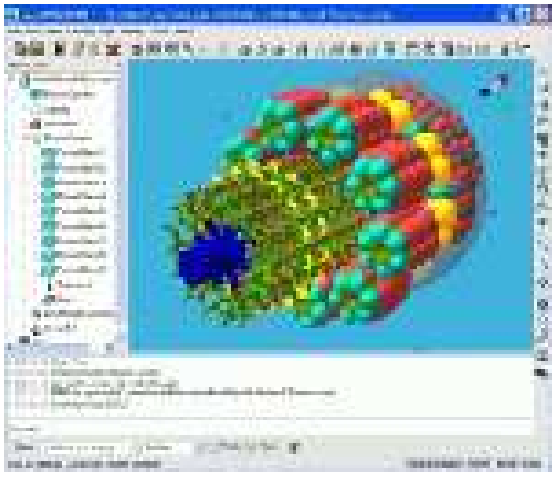
More new Tools will be ready for NanoEngineering Students in the Spring 2006...

Nanorex Inc. is the leading provider of computational modeling tools made specifically for the design and analysis of productive nanosystems. Nanorex's first product, nanoENGINEER-1™, is a 3D nanomechanical CAD program. It includes both a sophisticated CAD module for the design and modeling of atomically precise components and assemblies, and a molecular dynamics module for setting up and simulating mechanical nanodevices. nanoENGINEER-1 is currently under development and is scheduled for release in early 2006.

Mark Sims, President of NanoRex has been avidly working to get the program ready for students in mechanical engineering at the university level. The Beta testing has brought back good reports and Damian Gregory Allis Ph.D. has been using it successfully to develop new molecular motor graphics that can be viewed on his website gallery for a preview of the capabilities of this dynamic program. www.somewhereville.com
An in-depth interview with Dr. Allis about his experience with the tools is available at: http://www.nanoengineer1.com/mambo/index.php?option=com_content&task=view&id=108&Itemid=2



Marks Sims has stated that in order to build productive nanosystems, you first have to design them. To design them, you need a unique computer-aided nanodesign solution totally different from the available CAD and molecular modeling software used today. Many students just don't have access to this equipment. His goal has been to change all that and he works tirelessly to accomplish this feat. It must be easy to install and easy for students to use in the classrooms. The first programs will be offered free to educators and feedback from the classrooms will help in the final design process for a commercial program that can be sold globally.



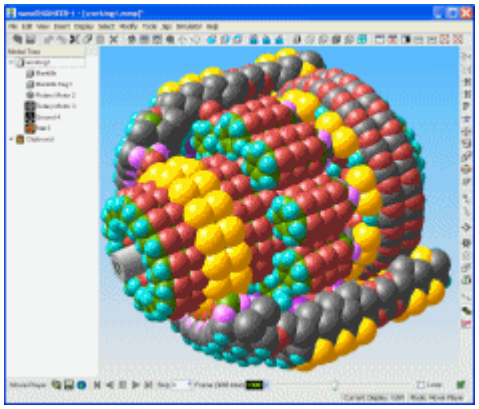
nanoENGINEER-1 has been developed with a familiar, intuitive user interface for mechnical engineers with experience using CAD programs like pro/ENGINEER or AutoCAD. nanoENGINEER-1 doesn't even require the user to know much about chemistry to use it. In fact, nanoENGINEER-1 is an excellent way for mechanical engineers to learn chemistry.

nanoENGINEER-1's molecular design module combines capabilities found in

traditional chemistry modeling software with features found in popular 3-D mechanical CAD systems. With nanoENGINEER-1, users can design atomically precise assemblies from a variety of stiff covalent structures, including a number of diamond-lattice frameworks. A parts library of molecular components is also included containing tubes, shafts, bearings, gears, joints, and springs that can be easily inserted and integrated with an existing assembly.

nanoENGINEER-1 MD Simulator

In addition, nanoENGINEER-1 includes a molecular dynamics module with motors, grounds and dampers that can be attached to a model to create interactive movies of molecular simulations. These movies can be played in forward or reverse, allowing the user to inspect the simulation results graphically at any point of the animation, from any angle. This tight coupling between design and simulation allows for rapid prototyping, analysis, refinement and validation of theoretical nanosystem designs.

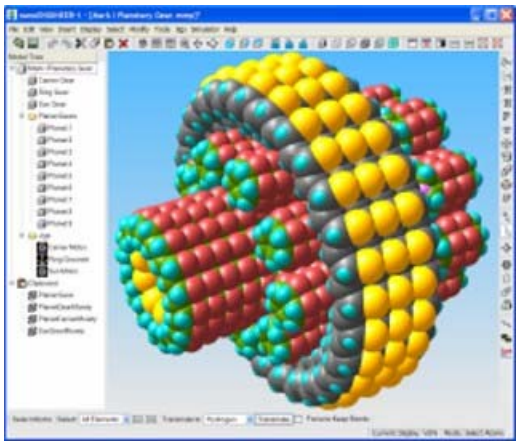
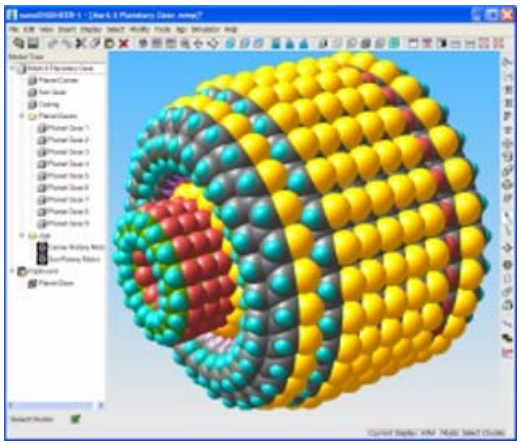


Mark III(k) Planetary GearOne of the first successful molecular dynamics simulations of the Mark III(k), a molecular planetary gear designed by Dr. K. Eric Drexler, was recently completed and added to the nanoENGINEER-1 Gallery.

The Mark III(k) gear is the result of multiple design iterations by Dr. Drexler, first in the early 1990s while writing the groundbreaking book Nanosystems: Molecular Machinery, Manufacturing, and Computation, and others done more recently. An early version of the gear is illustrated and described in detail on pages 311-312 of his book. That version, referred to as the Mark I, was a collaborative design with Dr. Ralph Merkle while working together at Xerox Palo Alto Research Center.

The Mark III series of planetary gear designs exploits symmetry properties involving the sun, planet, and ring gears to ensure smooth rotation. The planet gears have 6-fold symmetry, but in order to satisfy bonding constraints, this changes to 3-fold symmetry where they attach to the planet carrier. In earlier designs, these 3-fold parts interacted with the sun gear strongly enough to push the shaft noticeably off-axis. The Mark III(k) corrects this defect by separating the end of the sun gear from the 3-fold regions of the planet gears, and by making these 3-fold regions somewhat more compact.

The "k" in the name Mark III(k) comes from a series of file names of intermediate designs in the Mark III series, each involving a set of minor modifications, followed by minimization, examination and (until the last) revision.

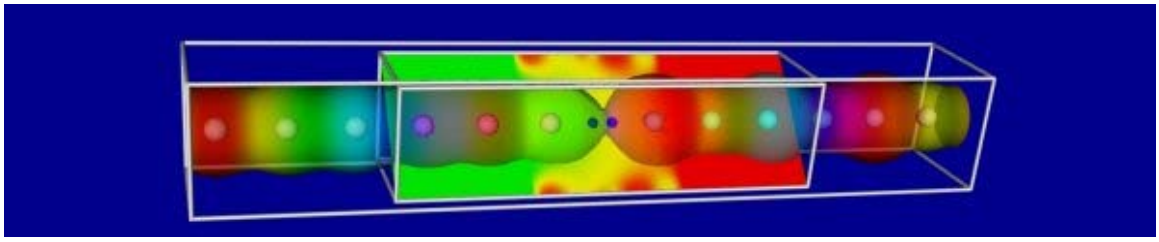



In between the Mark I and III series was the Mark II. It was the first design that had a closed casing, completed just after the first simulations of the Mark I by William Goddard's group at Cal Tech.

Academic Outreach Program

Nanorex is seeking academic institutions interested in using nanomechanical engineering software. Are you a university professor developing a nanoengineering course and would like to learn how students can use nanoENGINEER-1 to apply textbook theory in an educational setting? If so, send us an email at info@nanorex.com and find out about our Academic Outreach Program. If you qualify, you and your students will receive free packaged software and support. We can also assist you in developing a nanoengineering course syllabus including workbook exercises to teach students the process of designing, modeling and simulating nanomechanical devices.

For more information and to Request permission to Download the test copy of the software visit: http://www.nanoengineer-1.com/mambo/index.php



Atomistix of Denmark is the leading edge software for modeling the electrical properties of nanoscale devices. Well known in Europe and Asia, their tools resolve many issues for research involving nanoelectronics.

Co-founded by Thomas Magnussen, PhD, Kurt Stokbro, PhD and Jeremy Taylor, PhD, who is the main architect behind Atomistix' flagship product, The TranSIESTA-C package.

Kurt Stockbro also has 15 years of experience in the field of atomic-scale modeling software and is currently affiliated with the Nano-Science Center at Copenhagen University.

The trio, headed by Thomas Magnussen as CEO, form a dynamic team in their respective fields that are continuously expanding their field of vision for the global market.

Atomistix has developed a system of integrated software modules based on quantum theory - the Atomistix Virtual NanoLab™ - that can accurately calculate properties associated with electron distribution and transport, and simulate experiments with integrated nanoscale systems. The software is a unique tool to understand, predict and visualize electronic processes in atomic and molecular structures. With the software, nanotechnology scientists and engineers are able to establish competitive advantages by developing materials and designing products with radically new properties and functions.

Since incorporation in October 2003, the company has been working in close collaboration with the Nano-Science Center at the Niels Bohr Institute of Copenhagen University, for developing new quantum-chemical algorithms and an intuitive user interface in order to make these methods widely usable.

Atomistix is headquartered in Copenhagen, and has sold and distributed its software solutions on five continents. Atomistix offers support, training and consultancy to its users. The company is supporting its worldwide efforts with R & D and competence centres in Copenhagen and Singapore in cooperation with local scientific institutions. Atomistix is engaged in partnerships with leading marketing companies for distribution of the Atomistix Virtual NanoLab software throughout the globe.

A few of their recent projects include:

The Microelectronics Centre of the School of EEE (NTU) and Atomistix Asia Pacific Pte Ltd (AAP) has signed a 3-year Research Collaboration Agreement starting 1 February 2006, which amounts to ~S$2.2M in total from both parties (including ~S$500K incremental cash contribution to NTU by AAP), to embark on joint research and development in “bridging bottom-up atomic models with top-down compact modeling for future generation nanoelectronics circuit simulation”.

The joint project "Molecular Design with GRID Technology" of DIKU (Department of Computer Science, University of Copenhagen), DTU (Technical University of Denmark), the Nano-Science Center at the University of Copenhagen, MESH-Technologies A/S and Atomistix A/S has received a grant of DKK 8.6 million (USD 1.38 million) by the Danish Research Agency's Programme Commission on Nanoscience, Biotechnology and IT (NABIIT). This synthesis of leading grid computing and nanotechnology competence is expected to result in significant progress as well as new business opportunities within the field of chemi-informatics and atomic modeling.

If you are interested in their tools they have just released a new toolkit.

Atomistix ToolKit (ATK) 2.0 was released on February 7 2006 as the natural evolution of TranSIESTA-C.

ATK 2.0 represents a significant step towards our vision of creating a Virtual NanoLab, where advanced modeling of complex nanoscale systems is performed in an intuitive and yet highly flexible environment.

Among the vast array of features in ATK, we would like to highlight the following unique capabilities (* marks a new feature in ATK 2.0 compared to TranSIESTA-C):

Self-consistent first-principles description of molecules, periodic systems and two-probe structures, using density functional theory (DFT)with LDA and GGA-PBE exchange-correlation functionals.

Calculation of electronic transport properties of nanoscale systems, including transmisson spectrum, conductance and current-voltage characteristics at finite bias, through the use of non-equillibrium Green's function (NEGF).

Parallelized code, with almost linear scaling for certain types of heavy transport calculations. (*)

Ability to study spin-polarized transport and energy spectra in nanostructures. (*)
k-point sampling for transmission spectrum/current. (*)

Flexible yet simple text input format, allowing for specification of physical quantities in different units, relative or scaled coordinates, etc.
For product information visit their website.
http://www.atomistix.com

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Software solutions for Computational Science and Informatics in pharmaceuticals, chemicals and materials science.

Accelrys is a leader in scientific software solutions that help transform the discovery and development of innovative pharmaceuticals, chemicals and materials. Their Center of Excellence is located in San Diego with a global market serving corporate, academia and government organizations. With over twenty years of leadership in the delivery of computational science and informatics software to diverse R&D organizations, they work hard to execute their vision to transform the process of discovering and developing drugs and materials from experiment-driven to software-driven.

They have formed a scientific network to collaborate and partner actively with leading academic and industrial scientists, and other technology vendors. Over 200 PhD scientists maintain the products and innovate to extend and apply them. New science emerges via our product development, post-doctoral, sabbatical, and consortium programs.

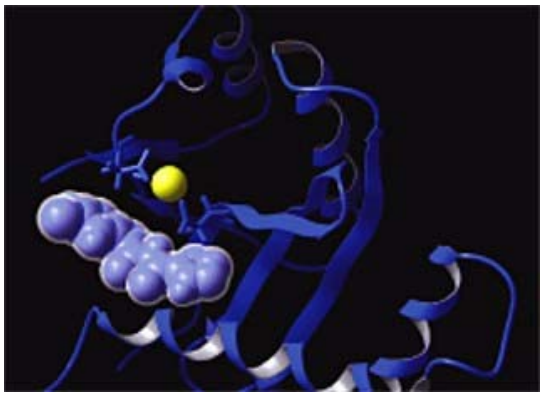
Solutions for Academic Researchers
Academic research is the lifeblood of the scientific community. Realizing this, we offer substantial reductions on software to academics. The information below will help introduce you to the solutions we have to enhance your research.

Products for Academic Researchers
We have identified a number of product sets that have proven to be of particular interest to academic researchers. These are summarized in our Software Solutions Brochure, which you can download as a PDF file at:
http://www.accelrys.com/solutions/academic/

For more solutions visit:
www.Accelrys.com

Chemistry 2005 Products of the Year Winner: MacroModel

I found this simulation software in Scientific Computer Magazine recently and had to include it as a solution for simulations in the classrooms.



MacroModel molecular modeling software is designed for general-purpose molecular mechanics for small and medium-sized organic molecules in both gas and solution phases, and includes utilities for exploring proteins and protein-ligand complexes.

It offers techniques for evaluating energy, sampling conformations and accounting for solvation of general molecular modeling of small organic molecules.

Made by Schrodinger, a scientific leader in developing state-of-the-art chemical simulation software for use in pharmaceutical and biotechnology research. Their products range from general molecular modeling to a full-featured suite of drug design software. Founded in 1990, Schrodinger has operations in New York, Oregon, and California, as well as Germany and England.

Visit their website for more information on products.
http://www.schrodinger.com/ProductDescription.php?mID=6&sID=8

Visualization tools for K-12 Classrooms

The only tool that is appropriate for developing K-12 education at this time is from Nano Science Instruments. They are the distributor in the United States and Canada for Nanosurf, the original developer of desktop scanners for education based in Switzerland. The new model just released has many options that are affordable and they are known for the ease-of-use by teachers, students and outreach programs for K-12.

The Nanosurf® EasyScan 2 AFM and STM
The Smart, Modular and Robust Scanning Probe Microscopes

Configure your own AFM or STM that suits your needs at an affordable cost.

The highly modular easyScan 2 line allows you to move from a very affordable STM system to a highly functional multiple mode AFM/STM package. You can configure what you need, or you can add options later.

The Swiss-made system is manufactured near the birthplace of the STM. High quality, precision machining, and a smart easy-to-use design makes the easyScan 2 the perfect choice for teaching or research where large STM and AFM microscopes are not practical or within budget for most classrooms.

Their website also features downloads for curriculum development tools, a list of outreach programs, an animation gallery and a quarterly newsletter with articles on the success of educational outreach programs for those considering the purchase of these tools.

Mark Flowers, President of Nanoscience Instruments is dedicated to education and has worked on project submissions with our group twice over the past 5 years. He recognizes the importance of teaching nano science in the primary grades and has been very helpful in providing resources that offer assistance to teachers in developing and disseminating information.

I have also included the animations from his gallery in many of my presentations around the world to encourage governments to initiate programs for K-12 curriculum in all development plans for funding nano science education. Young students will respond to these animated visual elements that show the atomic surfaces of graphite, platinum and other elements that are part of the underlying structure of matter. The ability to scan objects from nature that they recognize such as the skin on their hand, a fingernail, or a strand of hair for observation and clarity that “size does matter” in science will leave a lasting impression and create more desire to explore science as they mature.

The Windows applications on their website were written by Dr. Joe Griffith. They are provided as a convenience and come with no guarantee or support. The programs may not be redistributed for commercial purposes, as they are intended for evaluation of the respective products, while also offering valuable educational uses at no cost to you. Administrators and teachers can test these programs to develop expanded modules for their current science curriculum before the school districts budgets are prepared. http://www.nanoscience.com/education/software.html

This product was developed to enhance current curriculum in universities or K-12 education programs as a visual tool for expanding the knowledge base of our students while introducing them to science lab research experiences at an early age.

Nanoscience Instruments, Inc. is the exclusive distributor for Nanosurf in the U.S. & Canada. www.nanoscience.com Please contact them directly for pricing and delivery information within the U.S. & Canada and contact Nanosurf elsewhere for these products. www.nanosurf.com